On the linear representations of the symmetry groups of single-wall carbon nanotubes

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Abstract. The positions of atoms forming a carbon nanotube are usually described by using a system of generators of the symmetry group. Each atomic position corresponds to an element of the set $\mathbb{Z} \times \{0, 1, ..., n\} \times \{0, 1\}$, where n depends on the considered nanotube. We obtain an alternate rather different description by starting from a three-axes description of the honeycomb lattice. In our mathematical model, which is a factor space defined by an equivalence relation in the set $\big\{(v_0, v_1, v_2) \in \mathbb{Z}^3 \mid v_0 + v_1 + v_2 \in \{0, 1\}\big\}$, the neighbours of an atomic position can be described in a simpler way, and the mathematical objects with geometric or physical significance have a simpler and more symmetric form. We present some results concerning the linear representations of single-wall carbon nanotubes in order to illustrate the proposed approach.

1. Introduction

A single-wall carbon nanotube is a cylindrical structure with a diameter of a few nanometers, periodic along its axis, which can be imagined as a rolled up honeycomb lattice. The high symmetry of carbon nanotubes has facilitated the theoretical investigation of the physical phenomena occurring in these materials [1, 8, 9, 10, 12, 14]. The spatial symmetries (translations, rotations and screw axes, mirror and glide planes, etc.) form a line group, which is the maximal subgroup of the Euclidean group that leaves the nanotube invariant. The role of this group is analogous to that of crystallographic space groups in solid state physics. Some important properties of the band structure (electronic, phonon, etc.) can be directly deduced from the symmetry groups.

The symmetry group of a carbon nanotube depends on the diameter of the tubule and on the helical arrangement of the carbon hexagons. The irreducible representations of these groups are well-known [6, 7, 13], but, generally, equivalent representations offer distinct formal advantages. A calculation very simple in a representation can become much more complicated in an equivalent representation. Therefore, we think it is worth looking for new representations, and for new ways to describe the atomic structure of these materials. Our aim is to present an improved version of the mathematical model proposed in [3] and some applications illustrating this new approach.

2. Honeycomb lattice in a three-axes description

The vectors corresponding to the vertices of a regular triangle

$$e_0=(1,0),\qquad e_2=\left(-\frac{1}{2},\frac{\sqrt{3}}{2}\right),\qquad e_3=\left(-\frac{1}{2},-\frac{\sqrt{3}}{2}\right) \tag{1}$$

allow us to define the bijecton

$$\mathcal{L}\longrightarrow \mathbb{L}:\ (v_0,v_1,v_2)\mapsto v_0e_0+v_1e_1+v_2e_2 \tag{2}$$

from the set

$$\mathcal{L}=\{\ v=(v_0,v_1,v_2)\in\mathbb{Z}^3\ \mid\ v_0+v_1+v_2\in\{0;1\}\ \} \tag{3}$$

to the set $\mathbb{L}$ of all the vertices of a *honeycomb lattice.* The subset $\mathcal{L}$ of $\mathbb{Z}^3$ becomes in this way a mathematical model for the honeycomb lattice. One can remark that

$$\mathcal{L}=\mathcal{T}\cup(\mathcal{T}+(1,0,0)) \tag{4}$$

where

$$\mathcal{T}=\{\ v=(v_0,v_1,v_2)\in\mathbb{Z}^3\mid v_0+v_1+v_2=0\ \}. \tag{5}$$

The mapping

$$d:\mathcal{L}\times\mathcal{L}\longrightarrow\mathbb{N},\qquad d(v,u)=|v_0-u_0|+|v_1-u_1|+|v_2-u_2| \tag{6}$$

is a distance on $\mathcal{L}$, and u is a *neighbour of order* l of v if $d(v,u)=l$. The *nearest neighbours* of v are

$$\begin{array}{l} v^0=(v_0+\varepsilon(v),v_1,v_2)\\ v^1=(v_0,v_1+\varepsilon(v),v_2)\\ v^2=(v_0,v_1,v_2+\varepsilon(v)) \end{array} \qquad \text{where} \qquad \varepsilon(v)=(-1)^{v_0+v_1+v_2} \tag{7}$$

and the six *next-to-nearest neighbours* of v are the points $v^{ij}=(v^i)^j$ corresponding to all the pairs (i,j) with $i\neq j$. The *symmetry group* G of the honeycomb lattice coincides with the group of all the isometries of the metric space $(\mathcal{L},d)$, and is generated by the transformations

$$\begin{array}{ll} \mathcal{L}\longrightarrow\mathcal{L}: & (v_0,v_1,v_2)\mapsto(v_1,v_2,v_0)\\ \mathcal{L}\longrightarrow\mathcal{L}: & (v_0,v_1,v_2)\mapsto(v_0,v_2,v_1)\\ \mathcal{L}\longrightarrow\mathcal{L}: & (v_0,v_1,v_2)\mapsto(-v_0+1,-v_1,-v_2). \end{array} \tag{8}$$

The subgroup of *translations* contained in G corresponds to $\mathcal{T}$

$$\{\ u\ |\ v\in\mathcal{L}\Rightarrow v+u\in\mathcal{L}\ \}=\{\ u\in\mathcal{L}\ |\ \varepsilon(u)=1\ \}=\mathcal{T}. \tag{9}$$

We can extend the description based on e_0, e_1, e_2 to the whole plane. Each vector v admits the representation

$$v=a\sum_{i=0}^{2}\langle v,e_i\rangle e_i \qquad \text{with} \quad a=\frac{2}{3} \tag{10}$$

and the usual scalar product and norm become

$$\langle v,u\rangle=a\sum_{i=0}^{2}\langle v,e_i\rangle\langle u,e_i\rangle, \qquad ||v||=\sqrt{a\sum_{i=0}^{2}\langle v,e_i\rangle^2}. \tag{11}$$

The vectors e_0, e_1, e_2 form a tight frame [2] and a system of coherent vectors [4] in $\mathbb{R}^2$. For each vector v, the 'canonical coordinates'

$$\hat{v}_0=\langle v,e_0\rangle, \qquad \hat{v}_1=\langle v,e_1\rangle, \qquad \hat{v}_2=\langle v,e_2\rangle \tag{12}$$

satisfy the relation $\hat{v}_0+\hat{v}_1+\hat{v}_2=0$, and we can identify $\mathbb{R}^2$ with the space

$$\mathcal{K}=\{k=(k_0,k_1,k_2)\ |\ k_0,\ k_1,\ k_2\in\mathbb{R},\ k_0+k_1+k_2=0\ \} \tag{13}$$

by using the linear isomorphism

$$\mathcal{K}\longrightarrow\mathbb{R}^2:\ (k_0,k_1,k_2)\mapsto a\sum_{i=0}^{2}k_ie_i. \tag{14}$$

The representation of a vector v as a linear combination of e_0, e_1, e_2 is not unique

$$v=a\sum_{i=0}^{2}\hat{v}_i\,e_i=a\sum_{i=0}^{2}(\hat{v}_i+\alpha)e_i \tag{15}$$

for any $\alpha\in\mathbb{R}$. All the elements $(v_0,\ v_1,\ v_2)$ of the set

$$\{(\hat{v}_0+\alpha,\ \hat{v}_1+\alpha,\ \hat{v}_2+\alpha)\ |\ \alpha\in\mathbb{R}\ \}$$

correspond to the same point of the plane, and

$$\langle k, v\rangle = a\sum_{i=0}^{2} k_i\hat{v}_i = a\sum_{i=0}^{2} k_i(\hat{v}_i+\alpha) = a\sum_{i=0}^{2} k_i v_i \tag{16}$$

for all $k \in \mathcal{K}$.

3. An alternate mathematical model for carbon nanotubes

A *single-wall carbon nanotube* can be visualized as the structure obtained by rolling a honeycomb lattice (which is a mathematical model for a graphene sheet) such that the endpoints of a translation vector $c \in \mathcal{T}$ are folded one onto the other (see figure 1). The vector c is called the *chirality* of the tubule. After the graphene sheet rolling, the points ..., $v-2c$, $v-c$, v, $v+c$, $v+2c$, ... are folded one onto the other, for any $v \in \mathcal{L}$. Therefore, each element of the set $[v] = v + \mathbb{Z}c$, that is, each element of the set

$$[v_0, v_1, v_2] = \{\ (v_0, v_1, v_2) + j(c_0, c_1, c_2) \mid j \in \mathbb{Z}\ \} \tag{17}$$

describe the same point of the nanotube. The subset of the factor space $\mathbb{Z}^3/\mathbb{Z}c$

$$\mathcal{L}_c = \left\{\ [v_0, v_1, v_2] \in \frac{\mathbb{Z}^3}{\mathbb{Z}c}\ \middle|\ v_0 + v_1 + v_2 \in \{0; 1\}\ \right\} \tag{18}$$

can be regarded as a mathematical model for the nanotube of chirality c. A symmetry transformation $\mathcal{L} \longrightarrow \mathcal{L}:\ v \mapsto gv$ of the honeycomb lattice satisfying the relation

$$[v] = [u] \Longrightarrow [gv] = [gu] \tag{19}$$

defines a *symmetry transformation* of nanotube $\mathcal{L}_c$, namely

$$g : \mathcal{L}_c \longrightarrow \mathcal{L}_c : [v] \mapsto [gv]. \tag{20}$$

Each nanotube $\mathcal{L}_c$ admits the symmetry transformations:

$$\begin{array}{l} \tau : \mathcal{L}_c \longrightarrow \mathcal{L}_c : [v_0, v_1, v_2] \mapsto [-v_0+1, -v_1, -v_2] \\ g_u : \mathcal{L}_c \longrightarrow \mathcal{L}_c : [v] \mapsto [v+u] \qquad \text{for any} \qquad u \in \mathcal{T}. \end{array} \tag{21}$$

Let n be the greatest common divisor of c_0, c_1, c_2, and let $\tilde{c} = (\tilde{c}_0, \tilde{c}_1, \tilde{c}_2)$, where

$$\tilde{c}_0 = \frac{1}{n}c_0, \qquad \tilde{c}_1 = \frac{1}{n}c_1, \qquad \tilde{c}_2 = \frac{1}{n}c_2. \tag{22}$$

The transformation $g_{\tilde{c}}$ represents a *rotation of nanotube* of angle $2\pi/n$ with respect to its axis. Since

$$(c_2 - c_1)c_0 + (c_0 - c_2)c_1 + (c_1 - c_0)c_2 = 0 \tag{23}$$

the vector $(c_2 - c_1,\ c_0 - c_2,\ c_1 - c_0)$ is orthogonal to c (it has the direction of nanotube axis). The transformation g_t corresponding to

$$t = \frac{1}{\mathcal{R}}(c_2 - c_1,\ c_0 - c_2,\ c_1 - c_0) \tag{24}$$

where

$$\mathcal{R} = \gcd\{c_2 - c_1,\ c_0 - c_2,\ c_1 - c_0\} = \left\{ \begin{array}{lll} 3n & \text{if} & \tilde{c}_2 - \tilde{c}_1 \in 3\mathbb{Z} \\ n & \text{if} & \tilde{c}_2 - \tilde{c}_1 \not\in 3\mathbb{Z} \end{array} \right. \tag{25}$$

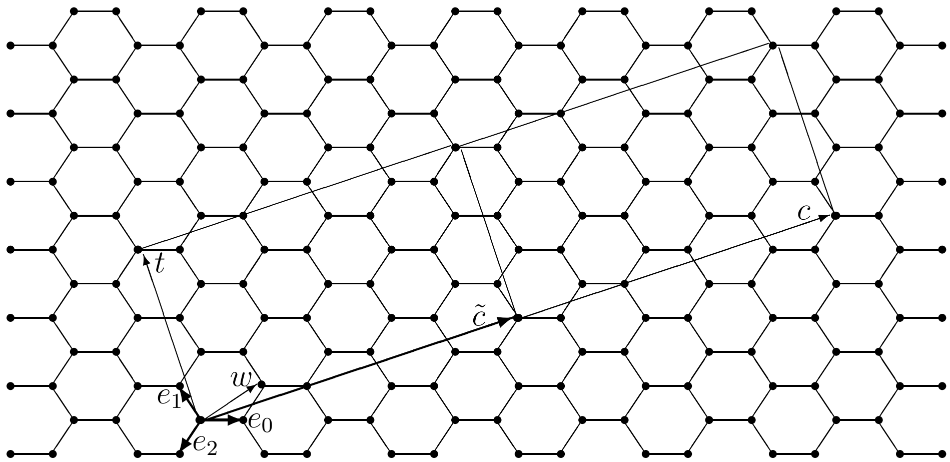

Figure 1. The unit cell of the carbon nanotube with the chiral vector $c = (10, -2, -8)$. In this case $n = 2$, $\tilde{c} = (5, -1, -4)$, $t = (-1, 3, -2)$, $w = (1, 0, -1)$ and $\tilde{q} = 14$.

represents the shortest pure translation of nanotube. From $c_0 + c_1 + c_2 = 0$ we get

$$(c_1 - c_2)^2 + (c_2 - c_0)^2 + (c_0 - c_1)^2 = 3(c_0^2 + c_1^2 + c_2^2) \tag{26}$$

that is, $\mathcal{R}^2||t||^2 = 3||c||^2$, whence

$$q = \frac{1}{\mathcal{R}}(c_0^2 + c_1^2 + c_2^2) \in n\mathbb{Z}. \tag{27}$$

For any $u \in \mathcal{T}$ the projections of u on c and t can be written

$$\frac{\langle u, c\rangle}{||c||^2}c = \left(u_1\frac{c_1 - c_0}{\mathcal{R}} + u_2\frac{c_2 - c_0}{\mathcal{R}}\right)\frac{c}{q}, \qquad \frac{\langle u, t\rangle}{||t||^2}t = \left(u_1\frac{c_2}{n} - u_2\frac{c_1}{n}\right)\frac{t}{\tilde{q}} \tag{28}$$

where $\tilde{q} = \frac{q}{n}$. Since

$$\gcd\{(c_1 - c_0)/\mathcal{R}, (c_2 - c_0)/\mathcal{R}\} = 1 \qquad \text{and} \qquad \gcd\{c_2/n, c_1/n\} = 1 \tag{29}$$

it follows that the projection of $\mathcal{T}$ on c is $\mathbb{Z}\frac{c}{q}$, and the projection of $\mathcal{T}$ on t is $\mathbb{Z}\frac{t}{\tilde{q}}$. Let $w \in \mathcal{T}$ be the shortest vector with

$$\frac{\langle w, t\rangle}{||t||^2}t = \frac{t}{\tilde{q}}. \tag{30}$$

From the relation

$$w = \frac{\langle w, c\rangle}{||c||^2}c + \frac{\langle w, t\rangle}{||t||^2}t \tag{31}$$

we get $[qw] = [nt]$.

Without lost of generality we can assume $c_0 > c_1 \geq c_2$. In the case $c_1 = c_2$ we have an *armchair* nanotube, and in the case $c_1 = 0$ a *zig-zag* nanotube. The nanotubes with $0 \neq c_1 \neq c_2$ are called *chiral nanotubes*. Our approach works for any single-wall carbon nanotube, but in this paper we restrict us to chiral nanotubes. The symmetry group G_c of the nanotube $\mathcal{L}_c$ is generated by the transformations $\varrho = g_{\tilde{c}}$, $\sigma = g_w$ and τ

$$G_c = \left\langle \varrho, \sigma, \tau \;\middle|\; \varrho\sigma = \sigma\varrho, \;\; \varrho^n = \tau^2 = (\sigma\tau)^2 = (\varrho\tau)^2 = e \right\rangle. \tag{32}$$

For each $[v] \in \mathcal{L}_c$ there exist $s \in \mathbb{Z}$, $m \in \{0, 1, ..., n-1\}$ and $p \in \{0;1\}$ uniquely determined such that $[v] = \sigma^s \varrho^m \tau^p [0,0,0]$. The usual description [5, 13] of the atomic positions of the atoms forming a carbon nanotube is based on this remark, and the set

$$\{(s,m,p) \mid s \in \mathbb{Z},\ m \in \{0,1,...,n-1\},\ p \in \{0,1\}\} \tag{33}$$

is used as a mathematical model. The alternate mathematical model we present in this paper is $\mathcal{L}_c$.

4. A tight-binding approach to carbon nanotubes

Consider the Hilbert space $(l^2(\mathcal{L}_c), \langle , \rangle)$, where

$$l^2(\mathcal{L}_c) = \left\{ \psi : \mathcal{L}_c \longrightarrow \mathbb{C} \;\middle|\; \sum_{v \in \mathcal{L}_c} |\psi(v)|^2 < \infty \right\} \tag{34}$$

$$\langle \psi_1, \psi_2 \rangle = \sum_{v \in \mathcal{L}_c} \overline{\psi_1(v)}\, \psi_2(v) \tag{35}$$

and the unitary representation of G_c in $l^2(\mathcal{L}_c)$ defined by

$$g : l^2(\mathcal{L}_c) \longrightarrow l^2(\mathcal{L}_c) \qquad (g\psi)[v] = \psi(g^{-1}[v]). \tag{36}$$

For each $\kappa \in (0, \infty)$, the linear operator

$$H : l^2(\mathcal{L}_c) \longrightarrow l^2(\mathcal{L}_c) \qquad (H\psi)[v] = \kappa \sum_{j=0}^{2} \psi[v^j] \tag{37}$$

is a self-adjoint G_c-invariant operator.

If $k \in \mathcal{K}$ is such that $\langle k, c \rangle \in 2\pi\mathbb{Z}$ then

$$\mathrm{e}^{\mathrm{i}\langle k,v \rangle} = \mathrm{e}^{\mathrm{i}\langle k,v+jc \rangle} \qquad \text{for any } \ j \in \mathbb{Z} \tag{38}$$

and hence, the function

$$\mathcal{L}_c \longrightarrow \mathbb{C} : \ [v] \mapsto \mathrm{e}^{-\mathrm{i}\langle k,v \rangle} \tag{39}$$

is well-defined (it does not depend on the representative we choose for $[v]$). The Hamiltonian used in the tight-binding description of π bands has the form (37).

Theorem 1. *a) For any k such that $\langle k, c \rangle \in 2\pi\mathbb{Z}$ the numbers $\pm E(k)$, where*

$$\begin{aligned} E(k) &= \kappa |\mathrm{e}^{\mathrm{i}k_0 a} + \mathrm{e}^{\mathrm{i}k_1 a} + \mathrm{e}^{\mathrm{i}k_2 a}| \\ &= \kappa \sqrt{3 + 2\cos(k_0 - k_1)a + 2\cos(k_1 - k_2)a + 2\cos(k_2 - k_0)a} \end{aligned} \tag{40}$$

belong to the spectrum of H.
b) The bounded functions belonging to an extension of $l^2(\mathcal{L}_c)$

$$\psi_k^{\pm} : \mathcal{L}_c \longrightarrow \mathbb{C}, \qquad \psi_k^{\pm}[v] = \mathrm{e}^{-\mathrm{i}\langle k,v \rangle} \varphi_k^{\pm}[v] \tag{41}$$

where

$$\varphi_k^{\pm}[v] = \left\{ \begin{array}{ccc} \mathrm{e}^{\mathrm{i}\lambda(k)} & if & \varepsilon(v) = 1 \\ \pm\mathrm{e}^{-\mathrm{i}\lambda(k)} & if & \varepsilon(v) = -1 \end{array} \right. \tag{42}$$

and

$$\lambda(k) = \begin{cases} -\frac{1}{2}\arg\left(\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}\right) & if \quad \mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a} \neq 0 \\ 0 & if \quad \mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a} = 0 \end{cases} \tag{43}$$

are eigenfunctions of H corresponding to the eigenvalues $\pm E(k)$, that is,

$$H\,\psi_k^\pm = \pm E(k)\,\psi_k^\pm. \tag{44}$$

Proof. a) The function $\psi : \mathcal{L}_c \longrightarrow \mathbb{C}$, $\psi[v] = \mathrm{e}^{-\mathrm{i}\langle k,v\rangle}\varphi[v]$, where

$$\varphi[v] = \begin{cases} \alpha & \text{if} \quad \varepsilon(v) = 1 \\ \beta & \text{if} \quad \varepsilon(v) = -1 \end{cases} \tag{45}$$

and α, β are two constants, satisfies the relation $H\psi = E\psi$ if and only if (α, β) is a solution of the system of equations

$$\begin{cases} \kappa(\mathrm{e}^{-\mathrm{i}k_0a} + \mathrm{e}^{-\mathrm{i}k_1a} + \mathrm{e}^{-\mathrm{i}k_2a})\beta = E\alpha \\ \quad \kappa(\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a})\alpha = E\beta. \end{cases} \tag{46}$$

This system has non-trivial solutions if and only if

$$\begin{vmatrix} -E & \kappa(\mathrm{e}^{-\mathrm{i}k_0a} + \mathrm{e}^{-\mathrm{i}k_1a} + \mathrm{e}^{-\mathrm{i}k_2a}) \\ \kappa(\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}) & -E \end{vmatrix} = 0 \tag{47}$$

that is, if and only if E is one of the numbers $\pm E(k)$.
b) If $\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_0a} \neq 0$ then the equation $\kappa(\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a})\alpha = \pm E(k)\beta$ leads to

$$\beta = \pm\alpha \frac{\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}}{|\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}|} = \pm\alpha\,\mathrm{e}^{-2\mathrm{i}\lambda(k)}. \tag{48}$$

Choosing $\alpha = \mathrm{e}^{\mathrm{i}\lambda(k)}$ we get $\beta = \pm\mathrm{e}^{-\mathrm{i}\lambda(k)}$, and hence, up to a multiplicative constant, the solution of $H\,\psi = \pm E(k)\,\psi$ is $\psi = \psi_k^\pm$. If $\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_0a} = 0$ then $E(k) = 0$, and the functions

$$\psi_k^\pm[v] = \mathrm{e}^{-\mathrm{i}\langle k,v\rangle} \begin{cases} 1 & \text{if} \quad \varepsilon(v) = 1 \\ \pm 1 & \text{if} \quad \varepsilon(v) = -1 \end{cases} \tag{49}$$

are eigenfunctions. ∎

The relation $\langle k, c\rangle \in 2\pi\mathbb{Z}$ defines a family of equidistant straight lines orthogonal to c with the distance between neighbouring lines equal to $2\pi/||c||$.

Theorem 2. *a) The function*

$$E : \mathcal{K} \longrightarrow [0, 3\kappa] \qquad E(k) = \kappa|\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}| \tag{50}$$

is even and periodic

$$E(k) = E(-k) \qquad E(k) = E(k+b_0) = E(k+b_1) = E(k+b_2) \tag{51}$$

where

$$b_0 = \left(\frac{4\pi}{3a}, -\frac{2\pi}{3a}, -\frac{2\pi}{3a}\right), \quad b_1 = \left(-\frac{2\pi}{3a}, \frac{4\pi}{3a}, -\frac{2\pi}{3a}\right), \quad b_2 = \left(-\frac{2\pi}{3a}, -\frac{2\pi}{3a}, \frac{4\pi}{3a}\right). \tag{52}$$

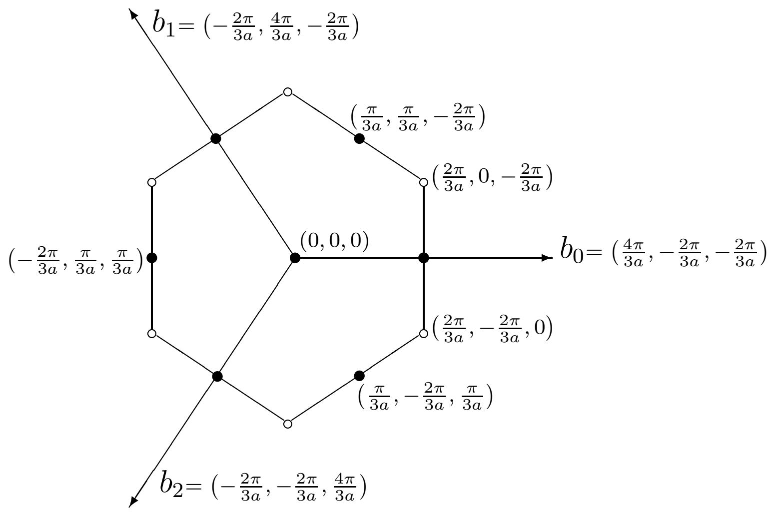

Figure 2. The hexagonal domain $\mathcal{B}$, the points of Λ (indicated by $\bullet$) and the points k with $E(k) = 0$, called K points (indicated by $\circ$).

b) The functions $\psi_k = \psi_k^+$ *and* ψ_k^- *are eigenfunctions of* ϱ *and* σ

$$\varrho\,\psi_k^\pm = \mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle}\,\psi_k^\pm \qquad\qquad \sigma\,\psi_k^\pm = \mathrm{e}^{\mathrm{i}\langle k,w\rangle}\,\psi_k^\pm \tag{53}$$

satisfy the relation

$$\tau\,\psi_k^\pm = \pm\mathrm{e}^{-\mathrm{i}k_0 a}\,\psi_{-k}^\pm. \tag{54}$$

c) The eigenspaces

$$\begin{array}{ll} \mathcal{E}_k & = \{\ \alpha\psi_k + \beta\psi_{-k}\ \ |\ \ \alpha,\ \beta\in\mathbb{C}\ \ \} \\ \mathcal{E}_k^- & = \{\ \alpha\psi_k^- + \beta\psi_{-k}^-\ \ |\ \ \alpha,\ \beta\in\mathbb{C}\ \ \} \end{array} \tag{55}$$

corresponding to $E(k)$ *and* $-E(k)$ *are* G_c*-invariant,* $\mathcal{E}_k = \mathcal{E}_{-k}$ *and* $\mathcal{E}_k^- = \mathcal{E}_{-k}^-$.
d) If k *is such that* $E(k) \neq 0$ *then*

$$\psi_{k+b_i}^\pm = \mathrm{e}^{\mathrm{i}\pi/3}\psi_k^\pm \qquad\qquad \mathcal{E}_{k+b_i} = \mathcal{E}_k \tag{56}$$

for any $i \in \{0, 1, 2\}$.

Proof. Since $\mathrm{e}^{\mathrm{i}4\pi/3} = \mathrm{e}^{-\mathrm{i}2\pi/3}$ we have

$$E(k+b_0) = \kappa\left|\mathrm{e}^{\mathrm{i}k_0a}\,\mathrm{e}^{\mathrm{i}4\pi/3} + \mathrm{e}^{\mathrm{i}k_1a}\,\mathrm{e}^{-\mathrm{i}2\pi/3} + \mathrm{e}^{\mathrm{i}k_2a}\,\mathrm{e}^{-\mathrm{i}2\pi/3}\right| = E(k).$$

$$\lambda(k+b_0) = -\frac{1}{2}\arg\left[\left(\mathrm{e}^{\mathrm{i}k_0a} + \mathrm{e}^{\mathrm{i}k_1a} + \mathrm{e}^{\mathrm{i}k_2a}\right)\mathrm{e}^{-\mathrm{i}2\pi/3}\right] = \lambda(k) + \frac{\pi}{3}$$

for any k with $E(k) \neq 0$. If v is such that $\varepsilon(v) = 1$ then $\langle b_0, v\rangle = 2\pi v_0$ and

$\psi_{k+b_0}[v] = \mathrm{e}^{-\mathrm{i}\langle k+b_0,v\rangle}\,\mathrm{e}^{\mathrm{i}\lambda(k+b_0)} = \mathrm{e}^{-\mathrm{i}\langle k,v\rangle}\,\mathrm{e}^{-\mathrm{i}2\pi v_0}\,\mathrm{e}^{\mathrm{i}\lambda(k)}\,\mathrm{e}^{\mathrm{i}\pi/3} = \mathrm{e}^{\mathrm{i}\pi/3}\,\psi_k[v].$

If v is such that $\varepsilon(v) = -1$ then $\langle b_0, v\rangle = 2\pi v_0 - 2\pi/3$ and

$\psi_{k+b_0}[v] = \mathrm{e}^{-\mathrm{i}\langle k+b_0,v\rangle}\,\mathrm{e}^{-\mathrm{i}\lambda(k+b_0)} = \mathrm{e}^{-\mathrm{i}\langle k,v\rangle}\,\mathrm{e}^{-\mathrm{i}2\pi v_0}\,\mathrm{e}^{\mathrm{i}2\pi/3}\mathrm{e}^{-\mathrm{i}\lambda(k)}\,\mathrm{e}^{-\mathrm{i}\pi/3} = \mathrm{e}^{\mathrm{i}\pi/3}\,\psi_k[v].$ ▪

From the periodicity of $E(k)$ and $\mathcal{E}_k$ it follows that we can restrict our analysis to the case $k \in \mathcal{B}_c$, where

$$\mathcal{B}_c = \{\ k \in \mathcal{B} \mid \ \langle k, c\rangle \in 2\pi\mathbb{Z}\ \} \tag{57}$$

and $\mathcal{B}$ is the hexagonal domain (see figure 2)

$$\mathcal{B} = \left\{ k \in \mathcal{K} \,\middle|\, -\frac{2\pi}{3a} \leq k_i \leq \frac{2\pi}{3a} \ \text{ for any } \ i \in \{0,1,2\} \right\}. \tag{58}$$

Theorem 3. *For even n the space $\mathcal{E}_k$ is one-dimensional if and only if $k \in \Lambda$, where*

$$\Lambda = \left\{ (0,0,0),\, \pm\left(-\frac{2\pi}{3a}, \frac{\pi}{3a}, \frac{\pi}{3a}\right),\, \pm\left(\frac{\pi}{3a}, -\frac{2\pi}{3a}, \frac{\pi}{3a}\right),\, \pm\left(\frac{\pi}{3a}, \frac{\pi}{3a}, -\frac{2\pi}{3a}\right) \right\}.$$

Proof. If $\mathcal{E}_k$ is one-dimensional then there is a constant C such that

$$\psi_{-k}[v] = C\psi_k[v] \qquad \text{for any } \ v \in \mathcal{L}_c.$$

For $v = (0,0,0)$ we get $C = \mathrm{e}^{-2\mathrm{i}\lambda(k)}$. Therefore

$$\psi_{-k} = C\,\psi_k \quad \Longleftrightarrow \quad \begin{cases} \mathrm{e}^{2\mathrm{i}\langle k,v\rangle} = 1 & \text{if } \ \varepsilon(v) = 1 \\ \mathrm{e}^{2\mathrm{i}\langle k,v\rangle} = C^2 & \text{if } \ \varepsilon(v) = -1. \end{cases} \tag{59}$$

Particularly, we must have $\mathrm{e}^{2\mathrm{i}k_0 a} = \mathrm{e}^{2\mathrm{i}k_1 a} = \mathrm{e}^{2\mathrm{i}k_2 a}$. For $k \in \mathcal{B}$ this relation is possible only if there are $\alpha, \beta \in \{0, \pm 1\}$ such that $k_1 = k_0 + \alpha\pi/a$ and $k_2 = k_0 + \beta\pi/a$. From $k_0 + k_1 + k_2 = 0$ we get

$$k = \left(-\frac{\alpha+\beta}{3}\frac{\pi}{a}, \frac{2\alpha-\beta}{3}\frac{\pi}{a}, \frac{-\alpha+2\beta}{3}\frac{\pi}{a} \right). \tag{60}$$

All these points points lie on the family of straight line defined by $\langle k, c\rangle \in 2\pi\mathbb{Z}$ since

$$\langle k, c\rangle = k_0 c_0 a + \left(k_0 + \alpha\frac{\pi}{a}\right) c_1 a + \left(k_0 + \beta\frac{\pi}{a}\right) c_2 a = (\alpha c_1 + \beta c_2)\pi \in 2\pi\mathbb{Z}. \tag{61}$$

In the case $\alpha = \beta = 0$ we get $k = (0,0,0)$, $\psi_k[v] = 1$, and

$$\varrho\psi_k = \psi_k \qquad \sigma\psi_k = \psi_k \qquad \tau\psi_k = \psi_k. \tag{62}$$

In the case $\alpha = \beta = 1$ we get $k = (-2\pi/3a, \pi/3a, \pi/3a)$, $\psi_k[v] = (-1)^{v_0}\mathrm{e}^{-\mathrm{i}\pi/6}$, and

$$\varrho\psi_k = (-1)^{\tilde{c}_0}\psi_k \qquad \sigma\psi_k = (-1)^{w_0}\psi_k \qquad \tau\psi_k = -\psi_k. \tag{63}$$

All the other points $k \in \mathcal{B}_c$ with $\dim \mathcal{E}_k = 1$ can be obtained from the analyzed points by using permutations of coordinates and/or a multiplication by (-1). ∎

In the case when n is odd only a part of the points of Λ lies on the family of straight lines defined by $\langle k, c\rangle \in 2\pi\mathbb{Z}$.

5. Two-dimensional representations of G_c

If $k\in\mathcal{B}_c\backslash\Lambda$ then $\dim\mathcal{E}_k=2$ and the matrices of ϱ, σ and τ in the basis $\{\psi_k,\,\psi_{-k}\}$ are

$$\varrho=\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle}\end{array}\right),\qquad \sigma=\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,w\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,w\rangle}\end{array}\right),\qquad \tau=\left(\begin{array}{cc}0 & \mathrm{e}^{\mathrm{i}k_0a}\\ \mathrm{e}^{-\mathrm{i}k_0a} & 0\end{array}\right) \tag{64}$$

Theorem 4. *For each $k\in\mathcal{B}_c\backslash\Lambda$ the representations of G_c in $\mathcal{E}_k$ and $\mathcal{E}_k^-$ are equivalent. They are reducible if and only if the numbers $\langle k,\tilde{c}\rangle$ and $\langle k,w\rangle$ belong to $\mathbb{Z}\pi$.*

Proof. The linear transformation $\mathcal{E}_k\longrightarrow\mathcal{E}_k^-\,:\,\alpha\psi_k+\beta\psi_{-k}\mapsto\mathrm{i}\alpha\psi_k^--\mathrm{i}\beta\psi_{-k}^-$ is an isomorphism of representations. If

$$P=\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right)$$

is the matrix in the basis $\{\psi_k,\,\psi_{-k}\}$ of the projector corresponding to a G_c-invariant subspace of $\mathcal{E}_k$ then $P^2=P$ and

$$\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right)\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle}\end{array}\right)=\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle}\end{array}\right)\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right) \tag{65}$$

$$\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right)\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,w\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,w\rangle}\end{array}\right)=\left(\begin{array}{cc}\mathrm{e}^{\mathrm{i}\langle k,w\rangle} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,w\rangle}\end{array}\right)\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right) \tag{66}$$

$$\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right)\left(\begin{array}{cc}0 & \mathrm{e}^{\mathrm{i}k_0a}\\ \mathrm{e}^{-\mathrm{i}k_0a} & 0\end{array}\right)=\left(\begin{array}{cc}0 & \mathrm{e}^{\mathrm{i}k_0a}\\ \mathrm{e}^{-\mathrm{i}k_0a} & 0\end{array}\right)\left(\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right). \tag{67}$$

From the last three relations it follows that

$$\beta\mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle}=\beta\mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle}\qquad \beta\mathrm{e}^{\mathrm{i}\langle k,w\rangle}=\beta\mathrm{e}^{-\mathrm{i}\langle k,w\rangle}\qquad \alpha\mathrm{e}^{\mathrm{i}k_0a}=\delta\mathrm{e}^{\mathrm{i}k_0a} \tag{68}$$

$$\gamma\mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle}=\gamma\mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle}\qquad \gamma\mathrm{e}^{\mathrm{i}\langle k,w\rangle}=\gamma\mathrm{e}^{-\mathrm{i}\langle k,w\rangle}\qquad \beta\mathrm{e}^{-\mathrm{i}k_0a}=\gamma\mathrm{e}^{\mathrm{i}k_0a}. \tag{69}$$

Since $\mathrm{e}^{\mathrm{i}k_0a}\neq 0$ we obtain $\alpha=\delta$. If either $\langle k,\tilde{c}\rangle\not\in\mathbb{Z}\pi$ or $\langle k,w\rangle\not\in\mathbb{Z}\pi$ then $\beta=\gamma=0$ and the representation (64) is irreducible. If the numbers $\langle k,\tilde{c}\rangle$ and $\langle k,w\rangle$ belong to $\mathbb{Z}\pi$ then imposing the condition $P^2=P$ we obtain

$$P=\frac{1}{2}\left(\begin{array}{cc}1 & \mathrm{e}^{\mathrm{i}k_0a}\\ \mathrm{e}^{-\mathrm{i}k_0a} & 1\end{array}\right)\qquad\text{or}\qquad P=\frac{1}{2}\left(\begin{array}{cc}1 & -\mathrm{e}^{\mathrm{i}k_0a}\\ -\mathrm{e}^{-\mathrm{i}k_0a} & 1\end{array}\right). \tag{70}$$

These complementary projectors correspond to the decomposition

$$\mathcal{E}_k=\{\alpha(\psi_k+\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})\mid\alpha\in\mathbb{C}\,\}\oplus\{\alpha(\psi_k-\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})\mid\alpha\in\mathbb{C}\,\} \tag{71}$$

of $\mathcal{E}_k$ into direct sum of one-dimensional G_c-invariant subspaces, and

$$\varrho(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})=(-1)^m(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})$$

$$\sigma(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})=(-1)^p(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})$$

$$\tau(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})=\pm(\psi_k\pm\mathrm{e}^{-\mathrm{i}k_0a}\psi_{-k})$$

where $m,\, p \in \mathbb{Z}$ are such that $\langle k, \tilde{c}\rangle = m\pi$ and $\langle k, w\rangle = p\pi$. ▪

The relations (64) define for each k belonging to the set

$$\mathcal{B}_c^{irred} = \{\ k \in \mathcal{B}_c \backslash \Lambda \mid \langle k, \tilde{c}\rangle \notin \mathbb{Z}\pi \ \ \text{or} \ \ \langle k, w\rangle \notin \mathbb{Z}\pi\ \} \tag{72}$$

a two-dimensional irreducible representation $\mathcal{D}_c(k)$. Some of these representations are equivalent. Particularly, $\mathcal{D}_c(k) = \mathcal{D}_c(-k)$.

6. Clebsch-Gordan coefficients

Let $k,\, k' \in \mathcal{B}_c^{irred}$ be such that $k^+ = k + k'$ and $k^- = k - k'$ belong to $\mathcal{B}_c^{irred}$. The direct product of the representations $\mathcal{D}_c(k)$ and $\mathcal{D}_c(k')$ admits the decomposition

$$\mathcal{D}_c(k) \otimes \mathcal{D}_c(k') = \mathcal{D}_c(k^+) \oplus \mathcal{D}_c(k^-)$$

and the matrices corresponding to ϱ, σ and τ are

$$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k,\tilde{c}\rangle} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,\tilde{c}\rangle} \end{pmatrix} \otimes \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k',\tilde{c}\rangle} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\langle k',\tilde{c}\rangle} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k^+,\tilde{c}\rangle} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\langle k^-,\tilde{c}\rangle} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^-,\tilde{c}\rangle} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^+,\tilde{c}\rangle} \end{pmatrix}$$

$$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k,w\rangle} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\langle k,w\rangle} \end{pmatrix} \otimes \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k',w\rangle} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\langle k',w\rangle} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k^+,w\rangle} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\langle k^-,w\rangle} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^-,w\rangle} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^+,w\rangle} \end{pmatrix}$$

$$\begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}k_0 a} \\ \mathrm{e}^{-\mathrm{i}k_0 a} & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}k'_0 a} \\ \mathrm{e}^{-\mathrm{i}k'_0 a} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}k_0^+ a} \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_0^- a} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k_0^- a} & 0 & 0 \\ \mathrm{e}^{-\mathrm{i}k_0^+ a} & 0 & 0 & 0 \end{pmatrix} \tag{73}$$

respectively. The unitary matrix

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{74}$$

satisfies the relations

$$M^{-1} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k^+,\tilde{c}\rangle} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\langle k^-,\tilde{c}\rangle} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^-,\tilde{c}\rangle} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^+,\tilde{c}\rangle} \end{pmatrix} M = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\langle k^+,\tilde{c}\rangle} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\langle k^+,\tilde{c}\rangle} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\langle k^-,\tilde{c}\rangle} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}\langle k^-,\tilde{c}\rangle} \end{pmatrix}$$

$$M^{-1}\begin{pmatrix} e^{i\langle k^+,w\rangle} & 0 & 0 & 0 \\ 0 & e^{i\langle k^-,w\rangle} & 0 & 0 \\ 0 & 0 & e^{-i\langle k^-,w\rangle} & 0 \\ 0 & 0 & 0 & e^{-i\langle k^+,w\rangle} \end{pmatrix} M = \begin{pmatrix} e^{i\langle k^+,w\rangle} & 0 & 0 & 0 \\ 0 & e^{-i\langle k^+,w\rangle} & 0 & 0 \\ 0 & 0 & e^{i\langle k^-,w\rangle} & 0 \\ 0 & 0 & 0 & e^{-i\langle k^-,w\rangle} \end{pmatrix}$$

$$M^{-1}\begin{pmatrix} 0 & 0 & 0 & e^{ik_0^+a} \\ 0 & 0 & e^{ik_0^-a} & 0 \\ 0 & e^{-ik_0^-a} & 0 & 0 \\ e^{-ik_0^+a} & 0 & 0 & 0 \end{pmatrix} M = \begin{pmatrix} 0 & e^{ik_0^+a} & 0 & 0 \\ e^{-ik_0^+a} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ik_0^-a} \\ 0 & 0 & e^{-ik_0^-a} & 0 \end{pmatrix}. \tag{75}$$

Therefore, the entries of M are Clebsch-Gordon coefficients [11] corresponding to the considered direct product. In this case, the only non-null coefficients are

$$(kk'11|k^+1) = (kk'12|k^-1) = (kk'21|k^-2) = (kk'22|k^+2) = 1. \tag{76}$$

More details concerning the Clebsch-Gordon coefficients and their applications in carbon nanotube physics can be found in the articles of Damnjanović et al. [5, 7, 13].

7. Concluding remarks

The present paper can be regarded as a pure mathematical exercise. We have defined the factor sets $\mathcal{L}_c$, the groups G_c acting on $\mathcal{L}_c$ as groups of permutations, and we have studied certain representations of these groups defined on some spaces of functions $\psi : \mathcal{L}_c \longrightarrow \mathbb{C}$. We have proved that the groups G_c are isomorphic to the symmetry groups of single-wall carbon nanotubes, and the considered representations are directly related to some representations used in carbon nanotube physics.

The present paper can also be regarded as presenting an alternate mathematical model for carbon nanotubes. We think that this alternate approach offers some formal advantages, namely, certain calculations may be simpler in this approach than in the usual one.

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References

[1] Ajiki H and Ando T 1993 Electronic states of carbon nanotubes *J. Phys. Soc. Japan* **62** 1255–66

[2] Andersson L M , Åberg J, Karlsson H O and Goscinski O 2002 Properties of a discretized coherent state representation and the relation to Gabor analysis *J. Phys. A: Math. Gen.* **35** 7787-801

[3] Cotfas N 2005 An alternate mathematical model for single-wall carbon nanotubes *J. Geom. Phys.* **55** 123–34, `http://fpcm5.fizica.unibuc.ro/~ncotfas`

[4] Cotfas N 2000 Systems of coherent vectors *J. Phys. A: Math. Gen.* **33** 5003–9

[5] Damnjanović M, Milošević I, Vuković T and Marinković T 2004 Wigner-Eckart theorem in the inductive spaces and applications to optical transitions in nanotubes *J. Phys. A: Math. Gen.* **37** 4059–68

[6] Damnjanović M, Milošević, Vuković T and Maultzsch J 2003 Quantum numbers and band topology of nanotubes *J. Phys. A: Math. Gen.* **36** 5707–17

[7] Damnjanović M, Milošević, Vuković T, Nikolić and Dobardžić 2002 Symmetry and electro-optical properties of nanotubes *Internat. J. Nanosci.* **1** 313-25

[8] Dresselhaus M S , Dresselhaus G and Eklund P C 1998 *Science of Fullerenes and Carbon Nanotubes* (San Diego, CA: Academic)

[9] Hamada H, Sawada S and Oshiyama A 1992 New one-dimensional conductors: graphitic microtubules *Phys. Rev. Lett.* **68** 1579–81

[10] Jishi R, Venkataraman L, Dresselhaus M S and Dresselhaus G 1995 Symmetry properties of chiral carbon nanotubes *Phys. Rev. B* **51** 11176–9

[11] Kibler M 1997 Symmetries in nuclear, atomic and molecular spectroscopy *Symmetries in Physics* ed F Gieres *et al* (Paris: Editions Frontières) 33-62

[12] Saito R, Dresselhaus G and Dresselhaus M 1998 *Physical Properties of Carbon Nanotubes* (London: Imperial College Press)

[13] Vuković T, Milošević I and Damnjanović M 2002 Carbon nanotubes band assignation, topology, Bloch states, and selection rules *Phys. Rev. B* **65** 045418

[14] White C T, Robertson D H and Mintmire J W 1993 Helical and rotational symmetries of nanoscale graphitic tubules *Phys. Rev. B* **47** 5485–8